

IN THE CLAIMS

Please amend the claims as follows:

Claim 1 (Currently Amended): A method for mining mass spectra, comprising:  
providing an input mechanism for a user to input specifying spectral characteristics of  
to be identified in a mass spectrum to be mined; and for said user to input specifying a  
relationship between said spectral characteristics ~~of said mass spectrum to be mined;~~  
receiving from said input mechanism user input spectral characteristics to be used to  
identify said spectral characteristics in said mass spectrum to be mined;  
receiving from said input mechanism a user input relationship indicative of said  
relationship between said spectral characteristics;  
searching said mass spectrum to be mined for portions ~~of said mass spectrum~~ which  
match said spectral characteristics based on said user input relationship; and  
assigning scores to said portions of said mass spectrum to be mined to indicate a  
degree of correlation between said portions of said mass spectrum to be mined and said  
spectral characteristics.

Claim 2 (Previously Presented): The method of claim 1, wherein said mass spectrum  
is obtained by any one of dissociation and full-scan.

Claim 3 (Original): The method of claim 1, wherein the step of specifying spectral  
characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

Claim 4 (Original). The method of claim 1, wherein  
said step of specifying a relationship includes identifying each of said spectral  
characteristics as being one of a primary and a secondary spectral characteristic, said

secondary spectral characteristic being linked hierarchically with said primary spectral characteristic and detected only after said primary spectral characteristic is detected.

Claim 5 (Previously Presented): The method of claim 3, wherein  
said step of specifying at least one of a product ion, a loss ion, and an ion series  
comprises specifying each of a product ion, a loss ion, and an ion series; and  
said assigning step includes:

- calculating a product ion score;
- calculating a loss ion score;
- calculating an ion series score;
- adjusting said product ion, loss ion, or said ion series score if respective said  
product ion, loss ion, or ion series spectral characteristic is secondary; and
- adding said product ion, loss ion, and ion series scores.

Claim 6 (Original): The method of claim 5, wherein the step of calculating a product  
ion score includes:

- identifying a most abundant ion within a window around said product ion spectral  
characteristic; and
- setting said product ion score as a percentage of total ion current of said identified ion.

Claim 7 (Original): The method of claim 5, wherein the step of calculating a loss ion  
score includes: calculating a loss ion mass per unit charge based on an actual precursor ion  
mass per unit charge and said loss ion spectral characteristic;

- identifying a most abundant ion within a window around said calculated loss ion mass  
per unit charge; and

setting said loss ion score as a percentage of total ion current of said identified ion.

Claim 8 (Previously Presented): The method of claim 5, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;

generating hypothetical ions separated by said specified distances;

aligning said mass spectrum with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned mass spectrum at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \cdot \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 9 (Original): The method of claim 5, wherein said adjusting step includes:

setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

Claim 10 (Previously Presented): The method of claim 1, further comprising:

preprocessing said mass spectrum; and displaying said scores from said assigning step.

Claim 11 (Previously Presented): The method of claim 10, wherein said preprocessing step includes:

subtracting nonfragment ions from said mass spectrum;  
estimating a precursor charge of mass spectrum resulting from said subtracting step;  
and  
normalizing an ion intensity of said mass spectrum from said estimating step as a percentage of a total ion current.

Claim 12 (Original): The method of claim 10, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

Claim 13 (Previously Presented): The method of claim 1, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said mass spectrum, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said mass spectrum.

Claim 14 (Previously Presented): The method of claim 1, further comprising:  
adjusting control parameters of a device that produces said mass spectrum based on said assigned scores.

Claim 15 (Currently Amended): A method for mining collision-induced dissociation (CID) spectra, comprising:

providing an input mechanism for a user to input specifying spectral characteristics of to be identified in a CID spectrum to be mined; and for said user to input specifying a relationship between said spectral characteristics of said CID spectrum to be mined;

receiving from said input mechanism user input spectral characteristics to be used to identify said spectral characteristics in said mass spectrum to be mined;

receiving from said input mechanism a user input relationship indicative of said relationship between said spectral characteristics;

searching said CID spectrum to be mined for portions of said CID spectrum which match said spectral characteristics based on said user input relationship; and

assigning scores to said portions of said CID spectrum to be mined to indicate a degree of correlation between said portions of said CID spectrum to be mined and said spectral characteristics.

Claim 16 (Original): The method of claim 15, wherein the step of specifying spectral characteristics includes specifying at least one of a product ion, a loss ion, and an ion series.

Claim 17 (Original). The method of claim 15, wherein  
said step of specifying a relationship includes identifying each of said spectral characteristics as being one of a primary and a secondary spectral characteristic, said secondary spectral characteristic being linked hierarchically with said primary spectral characteristic and detected only after said primary spectral characteristic is detected

Claim 18 (Previously Presented): The method of claim 16, wherein

said step of specifying at least one of a product ion, a loss ion, and an ion series comprises specifying each of a product ion, a loss ion, and an ion series; and

said assigning step includes:

calculating a product ion score;

calculating a loss ion score;

calculating an ion series score;

adjusting said product ion, loss ion, or said ion series score if respective said product ion, loss ion, or ion series spectral characteristic is secondary; and

adding said product ion, loss ion, and ion series scores.

Claim 19 (Original): The method of claim 18, wherein the step of calculating a product ion score includes:

identifying a most abundant ion within a window around said product ion spectral characteristic; and

setting said product ion score as a percentage of total ion current of said identified ion.

Claim 20 (Original): The method of claim 18, wherein the step of calculating a loss ion score includes:

calculating a loss ion mass per unit charge based on an actual precursor ion mass per unit charge and said loss ion spectral characteristic;

identifying a most abundant ion within a window around said calculated loss ion mass per unit charge; and

setting said loss ion score as a percentage of total ion current of said identified ion.

Claim 21 (Previously Presented): The method of claim 18, wherein said step of calculating said ion series score includes:

specifying distances between ions in an ion series as the ion series spectral characteristic;

generating hypothetical ions separated by said specified distances;

aligning said CID spectrum with said hypothetical ions;

identifying most abundant ions within respective windows around said aligned CID spectrum at said specified distances; and

setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \cdot \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 22 (Original): The method of claim 18, wherein said adjusting step includes: setting said secondary spectral characteristic score as a geometric mean of a primary spectral characteristic score and said secondary spectral characteristic score,

wherein said secondary spectral characteristic score does not exceed said primary spectral characteristic score to which said secondary spectral characteristic score is linked.

Claim 23 (Previously Presented): The method of claim 15, further comprising: preprocessing said CID spectrum; and displaying said scores from said assigning step.

Claim 24 (Previously Presented): The method of claim 23, wherein said preprocessing step includes:

- subtracting nonfragment ions from said CID spectrum;
- estimating a precursor charge of said CID spectrum resulting from said subtracting step; and
- normalizing ion intensities of said CID spectrum from said estimating step as a percentage of a total ion current.

Claim 25 (Original): The method of claim 23, wherein the displaying step includes displaying said scores in one of tabular and graphical form.

Claim 26 (Previously Presented): The method of claim 15, wherein the step of specifying spectral characteristics includes automatically specifying said spectral characteristics based on said CID spectrum, and

wherein the step of specifying a relationship includes automatically specifying said relationship based on said CID spectrum.

Claim 27 (Previously Presented): The method of claim 15, further comprising:

adjusting control parameters of a device that produces said CID spectrum based on said assigned scores.

Claim 28 (Currently Amended): A system for mining mass spectra, comprising:

means for ~~specifying~~inputting by a user spectral characteristics ~~of to be identified in a~~ mass spectrum to be mined; and for inputting by the user ~~means for specifying a relationship~~ between said spectral characteristics ~~of said mass spectrum to be mined;~~



means for receiving user input spectral characteristics to be used to identify said spectral characteristics in said mass spectrum to be mined and for receiving a user input relationship indicative of said relationship between said spectral characteristics;

means for searching said mass spectrum to be mined for portions ~~of said mass spectrum~~ which match said spectral characteristics based on said user input relationship; and

means for assigning scores to said portions of said mass spectrum to be mined to indicate a degree of correlation between said portions of said mass spectrum to be mined and said spectral characteristics.

Claim 29 (Previously Presented): The system of claim 28, wherein said mass spectrum is obtained by any one of dissociation and full-scan.

Claim 30 (Previously Presented): The system of claim 28, further comprising:

means for preprocessing said mass spectrum; and

means for displaying said scores from said assigning means.

Claim 31 (Previously Presented): The system of claim 28, wherein the means for specifying spectral characteristics includes means for automatically specifying said spectral characteristics based on said mass spectrum, and

wherein the means for specifying a relationship includes means for automatically specifying said relationship based on said mass spectrum.

Claim 32 (Previously Presented): The system of claim 28, further comprising:

means for adjusting control parameters of a device that produces said mass spectrum based on said assigned scores.

Claim 33 (Currently Amended): A system, comprising:

an input mechanism for a user to input spectral characteristics to be identified in a mass spectrum to be mined and for said user to input a relationship between said spectral characteristics;

a memory device having embodied therein ~~a~~ mass spectrum to be mined; and  
a processor in communication with the memory device and the input mechanism, the processor configured to

receive from said input mechanism specify user input spectral characteristics  
~~of to be used to identify said spectral characteristics in~~ said mass spectrum to be mined,

receive from said input mechanism a user input specify a relationship  
indicative of said relationship between said spectral characteristics ~~of said mass spectra to be mined~~,

search said mass spectrum to be mined for portions ~~of said mass spectrum~~  
which match said spectral characteristics based on said user input relationship, and

assign scores to said portions of said mass spectrum to be mined to indicate a degree of correlation between said portions of said mass spectrum to be mined and said spectral characteristics.

Claim 34 (Currently Amended): A computer program product including a computer readable medium for mining mass spectrum, comprising:

a graphical user interface code configured to allow a user to input spectral characteristics ~~of to be identified in~~ a mass spectrum to be mined and to ~~specify input~~ a relationship between said spectral characteristics; and

a mining code configured to search said mass spectrum to be mined for portions of ~~said mass spectrum~~ matching said spectral characteristics based on ~~said~~ a user input relationship indicative of said relationship between said spectral characteristics, and to assign scores to said portions of said mass spectrum to be mined to indicate a degree of correlation between said portions of said mass spectrum to be mined and said spectral characteristics.

Claim 35 (Previously Presented): The computer program product of claim 34, wherein said mass spectrum are obtained by any one of dissociation and full-scan.

Claim 36 (Original). The computer program product of claim 34, wherein the graphical user interface code is configured

to accept at least one of a product ion, a loss ion, and an ion series as an input, identify said spectral characteristics as being one of a primary and a secondary spectral characteristic, and

link said secondary spectral characteristic with said primary spectral characteristic such that said secondary spectral characteristic is detected only after said primary spectral characteristic is detected

Claim 37 (Previously Presented): The computer program product of claim 34, wherein the graphical user interface code comprises:

a control window configured to input the spectral characteristics and the relationship between said spectral characteristics of said mass spectrum; and

a results window configured to display said scores of said mass spectrum.

Claim 38 (Previously Presented): The computer program product of claim 34,  
wherein

said at least one of a product ion, a loss ion, and an ion series comprises each of a  
product ion, a loss ion, and an ion series; and

the mining code is configured to

calculate a product ion score,

calculate a loss ion score,

calculate an ion series score,

adjust said product ion, loss ion, or said ion series score if respective said  
product ion, loss ion, or ion series spectral characteristic is secondary, wherein said  
secondary spectral characteristic score does not exceed said primary spectral  
characteristic score to which said secondary spectral characteristic score is linked, and  
add said product ion, loss ion, and ion series scores.

Claim 39 (Previously Presented): The computer program product of claim 38,  
wherein said mining code is further configured to

calculate the product ion score by identifying a most abundant ion within a window  
around said product ion spectral characteristic and setting said product ion score as a  
percentage of total ion current of said identified ion,

calculate the loss ion score by calculating a loss ion mass per unit charge based on an  
actual precursor ion mass per unit charge and said loss ion spectral characteristic, identifying  
a most abundant ion within a window around said calculated loss ion mass per unit charge,  
and setting said loss ion score as a percentage of total ion current of said identified ion, and

calculate the ion series score by specifying distances between ions in an ion series as  
the ion series spectral characteristic, generating hypothetical ions separated by said specified

distances, aligning said mass spectrum with said hypothetical ions, identifying most abundant ions within respective windows around said aligned mass spectrum at said specified distances, and setting said ion series score as a geometric mean of a percentage of total ion current of said identified ions,

wherein said ion series score includes the following

$$N(I_1 \cdot I_2 \cdot I_3 \cdot \dots \cdot I_n)^{1/n}$$

where N is a number of said identified ions that correspond to said hypothetical ions and  $I_1$ - $I_n$  are respective percentages of said total ion current of said identified ions.

Claim 40 (Previously Presented): The computer program product of claim 34, further comprising:

a preprocessing code configured to process said mass spectrum prior to mining in order to remove spurious mass spectra data.

Claim 41 (Previously Presented): The computer program product of claim 40, wherein the preprocessing code is configured to

subtract nonfragment ions from said mass spectrum,  
estimate a precursor charge of said mass spectrum resulting from said subtracting step, and

normalize an ion intensity of said mass spectrum from said estimating step as a percentage of a total ion current.

Claim 42 (Original): The computer program product of claim 37, wherein the graphical user interface code further comprises:

a product ion window configured to input said product ion spectral characteristic;

a loss ion window configured to input said loss ion spectral characteristic; and  
an ion series window configured to input said ion series spectral characteristic,  
wherein said product ion, loss ion, and ion series windows open when respective said  
spectral characteristics are selected in said control window.

Claim 43 (Original): The computer program product of claim 37, wherein said  
results window displays said scores in one of tabular and graphical form.

Claim 44 (Previously Presented): The computer program product of claim 34,  
wherein the graphical user interface code is configured to accept automatically specified said  
spectral characteristics and said relationship based on said mass spectrum.

Claim 45 (Previously Presented): The computer program product of claim 34, further  
comprising:

a control code configured to adjust control parameters of a device which generates  
said mass spectrum based on said assigned scores.

Claim 46 (Original): A computer readable medium containing program instructions  
for execution on a computer system, which when executed by the computer system, cause the  
computer system to perform the method recited in any one of claims 1 through 14.

Claim 47 (Currently Amended): A graphical user interface, comprising:

a control window configured to accept an input from a user, the input including  
spectral characteristics ~~of~~ to be identified in a mass spectrum to be mined and a relationship  
between said spectral characteristics; and

a results window configured to display scores of portions of said mass spectrum to be mined indicating ~~how well~~ a correlation between said mass spectrum portions match and said spectral characteristics based on user input spectral characteristics and a user input relationship indicative of said relationship between said spectral characteristics.

Claim 48 (Original): The graphical user interface of claim 47, wherein said results window displays said scores in one of tabular and graphical form.